

# A simple quantum model of spontaneous emission

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We present a very simple model of a spontaneous emission from a two-level atom, interacting with a field of a finite number of states. Such a process is often said to occur because of the large number of equally-probable states of environment. We show that in our model increasing the number of field states may and may not cause a practically permanent emission, depending on the details of the model. We also describe how irreversibility emerges with growing number of states. Mathematical tools are reduced to a necessary minimum and hopefully can be well understood by undergraduate students.

## I. INTRODUCTION

In the introductory course on classical thermodynamics, statistical thermodynamics is sometimes based on the concept of equally-probable microstates<sup>1</sup>. However, the microscopic mechanism which guarantees this equal probability is not discussed.

Following this path, spontaneous emission may be said to occur because there exists large (or even infinite) number of excited states of environment and only one excited state of the atom. It can be argued that all those states are equally probable and thus the equilibrium state is the atom in ground state and somehow excited environment. After presenting the model in Section II, in Section III we present an example of a system, where the permanent emission is absent no matter how many states of the environment there are.

On the other hand, in the typical academic course on quantum mechanics<sup>2</sup>, stationary problems constitute a major part. The only three places where dynamics appear are the definition of time evolution operator, description of two-state system and the time-dependent perturbation theory. The last is usually presented in a general way for arbitrary number of states. The example in which one could trace how the system properties change with varying number of states is missing. We give such an example in Section IV.

Thanks to the simplicity of the model, the approach is free of semi-classical arguments and does not involve approximate methods like the perturbation theory. Thus, the model illustrates how fundamental principles of quantum dynamics works in a system more complex than a two-level one and can become a part of an introductory course on quantum mechanics, making it a little more oriented on dynamics than usual. Intuition build on this model may be of a great value when learning more advanced topics, like open quantum systems or quantum field theory, where the huge or infinite number of states is an essential difficulty.

## II. BUILDING THE MODEL

We assume that at the initial moment, the system contains single atom in excited state and the environment in the ground state. By spontaneous emission we understand the following situation: *We prepare the atom in an excited state. We wait some time  $t_w$  and measure if the atom is still excited. We repeat this procedure many times for similar, but not identical  $t_w$ . We find that if  $t_w$  is long enough, the atom is usually de-excited.* Note, that this definition suits to the experimental reality. In particular,  $t_w$  is not the same in any two real measurements is obvious.

We number all (orthogonal) basis states of the system by  $|0\rangle, |1\rangle, \dots, |N\rangle$ . We assume that  $N$  is finite. Thus, the space of states is an  $(N+1)$ -dimensional vector space and the Hamiltonian is an  $(N+1) \times (N+1)$  Hermitian matrix (Hermiticity is required for the total probability to be conserved during time evolution).

We choose  $|0\rangle$  to denote the initial state (*i.e.* the state in which the atom is excited and the environment is in its ground state). The states  $|k\rangle$  with  $k > 0$  correspond to different types of excitation of environment. These types of excitations we call "modes", in reference to quantum optics. Notice, that all basis states are the states of the whole system, *i.e.* the atom and the environment. They differ in the part of the system, which is excited.

Now we would like to write down the Hamiltonian of the system, which allows the system to flow from the state  $|0\rangle$  to some state  $|k\rangle$ . In quantum mechanics time evolution of the system is described by the time-evolution operator  $U_t$ ,

$$|\psi(t)\rangle = U_t|\psi(0)\rangle = e^{iHt/\hbar}|\psi(0)\rangle. \quad (1)$$

With the spectral theorem, we immediately see that in the eigenbasis of  $H$  the operator  $U_t$  is a diagonal matrix with matrix elements

$$\langle e_n | U_t | e_{n'} \rangle = \delta_{nn'} e^{iE_n t/\hbar}, \quad (2)$$

where  $n, n' \in \{0, 1, \dots, N\}$ ,  $|e_n\rangle$  are eigenstates of  $H$ ,  $E_n$  are corresponding eigenvalues and  $\delta$  denotes the Kronecker delta. In arbitrary basis for small  $\Delta t$  we have

$$U_{\Delta t} \approx I + iH\Delta t/\hbar \quad (3)$$

and we see that if the Hamiltonian matrix element  $\langle k|H|0\rangle$  is non-zero,  $|\psi(t + \Delta t)\rangle$  has different component  $|k\rangle$  then  $|\psi(t)\rangle$ . Otherwise,  $\langle k|\psi(t + \Delta t)\rangle = \langle k|\psi(t)\rangle$ . This is valid for all  $t$ , so  $\langle k|H|0\rangle$  must be non-zero if evolution from  $|0\rangle$  directly to  $|k\rangle$  is possible. We denote  $\langle k|H|0\rangle = \alpha_k$ . Due to Hermiticity, also  $\langle 0|H|k\rangle = \alpha_k^*$  must be non-zero, so the reverse process is also possible. This is true for all  $k > 0$ .

We assume that different modes are independent, *i.e.* the Hamiltonian does not mix them,  $\langle k|H|k'\rangle = 0$  for  $k \neq k'$ . This assumption is not necessary, but simplifies the model. We denote  $\langle k|H|k\rangle$  ( $k \in \{0, 1, \dots, N\}$ ) by  $\varepsilon_k$ .

The probability that the atom is excited after time  $t$  is  $P(t) = |\langle 0|\psi(t)\rangle|^2$ . Using Eq. (1) and (2), we can write it as

$$P(t) = \left| \sum_{n=0}^N |\langle 0|e_n\rangle|^2 e^{iE_n t/\hbar} \right|^2. \quad (4)$$

### III. DESTROYING STEREOTYPES

Now we would like to describe with our model two systems, where the spontaneous emission is not present. They are counterexamples for some widespread stereotypes.

The first example is the case  $N = 1$  (there is only one excited state of environment),  $\varepsilon_1 = \varepsilon_0$  (mean energies of the state with excited atom and of the state with excited environment are the same) and arbitrary  $\alpha_1 = \alpha$ . Then  $H$  is  $2 \times 2$  matrix,

$$\begin{aligned} H_1 &= \varepsilon_0(|0\rangle\langle 0| + |1\rangle\langle 1|) + \alpha|0\rangle\langle 1| + \alpha^*|1\rangle\langle 0| \\ &= \begin{bmatrix} \varepsilon_0 & \alpha \\ \alpha^* & \varepsilon_0 \end{bmatrix}. \end{aligned} \quad (5)$$

It is easy to compute eigenvalues and eigenstates from characteristic equation. Then from Eq. (4) follows

$$P_1(t) = \cos^2\left(\frac{|\alpha|t}{\hbar}\right). \quad (6)$$

This means that no spontaneous emission is present. The atom oscillates between the ground and the excited states. We can say it is at resonance with the field. Students can individually check that similar result holds for arbitrary  $\varepsilon_1$  (*i.e.* out of resonance), but the amplitude of oscillation is smaller and the atom is never certainly de-excited.

This example is a special case of the familiar 2-level system. It destroys the stereotype, that "going to lower energy" is prescribed in any quantum theory.

As the second example we consider the case of  $N$  identical states, *i.e.*  $\varepsilon_k = \varepsilon_0$  and  $\alpha_k = \alpha$ , for some given  $N$ . The Hamiltonian now has the form

$$H_2 = \varepsilon_0 \sum_{k=0}^N |k\rangle\langle k| + \sum_{k=1}^N (\alpha|0\rangle\langle k| + \alpha^*|k\rangle\langle 0|). \quad (7)$$

This example can be solved analytically by a simple change of the basis. We denote

$$|\tilde{1}\rangle = \frac{1}{\sqrt{N}} \sum_{k=1}^N |k\rangle. \quad (8)$$

The new basis consists of  $|\tilde{0}\rangle = |0\rangle$ ,  $|\tilde{1}\rangle$ , and any orthogonal to them (and each other) and normalized states  $|\tilde{2}\rangle, \dots, |\tilde{N}\rangle$ . The part of Hamiltonian proportional to the identity matrix  $\sum_{k=0}^N |k\rangle\langle k|$  looks the same in any basis. Using Eq. (8) and the facts that  $\langle 0|\tilde{k}\rangle = 0$  is the condition of orthogonality to  $|\tilde{0}\rangle$  and  $\sum_{k=1}^N \langle k|\tilde{k}\rangle = 0$  is the condition of orthogonality to  $|\tilde{1}\rangle$ , the following part can be expressed as

$$\begin{aligned} \sum_{k=1}^N \alpha|0\rangle\langle k| + h.c. &= \sum_{k=1}^N \sum_{\tilde{k}=\tilde{0}}^{\tilde{N}} \alpha|0\rangle\langle k|\tilde{k}\rangle\langle \tilde{k}| + h.c. \\ &= \sqrt{N}\alpha|0\rangle\langle \tilde{1}| + h.c. \end{aligned} \quad (9)$$

(*h.c.* denotes "Hermitian conjugate"). Thus all states orthogonal to  $|\tilde{0}\rangle$  and  $|\tilde{1}\rangle$  are eigenstates with eigenvalue  $\varepsilon_0$ . This means that we only have to find two last eigenstates, *i.e.* diagonalize remaining  $2 \times 2$  submatrix. Further calculation and the resulting evolution is similar to the case  $N = 1$ . The probability that the atom is excited is

$$P_2(t) = \cos^2\left(\frac{\sqrt{N}|\alpha|t}{\hbar}\right). \quad (10)$$

No spontaneous emission is present, no matter how large  $N$  is. This example destroys the stereotype that microstates are always equally probable and the huge number of possible states affirm that spontaneous emission is present in the system.

### IV. CONDITIONS FOR SPONTANEOUS EMISSION

To understand when spontaneous emission occurs we analyse Eq. (4). We notice that the expression for  $P(t)$  resembles a bit a square of module of some Fourier series. Consider the special case when  $N = 2M$ . To parametrize eigenvalues and eigenstates we use  $m \in \{-M, \dots, M\}$  instead of  $n \in \{0, \dots, 2M\}$ . We assume that the eigenvalues are equally-spaced in the section  $\varepsilon_0 \pm D$ ,

$$E_m = \varepsilon_0 + \frac{m}{M}D, \quad (11)$$

and that

$$\langle 0|e_m\rangle = \langle 0|e_{-m}\rangle. \quad (12)$$

We would like to stress, that now we make assumptions about the eigenvalues of the whole system and we have not yet discussed the Hamiltonian matrix elements  $\varepsilon_k$  and  $\alpha_k$  in our initial basis.

From Eq. (4) we have

$$\begin{aligned}\sqrt{P_3(t)} &= \left| e^{i\varepsilon_0 t/\hbar} \sum_{m=-M}^M |\langle 0|\tilde{e}_m\rangle|^2 e^{i\frac{m}{M}Dt/\hbar} \right| \\ &= \left| |\langle 0|\tilde{e}_0\rangle|^2 + \sum_{m=1}^M 2|\langle 0|\tilde{e}_m\rangle|^2 \cos\left(i\frac{m}{M}Dt/\hbar\right) \right|.\end{aligned}\quad (13)$$

Eq. (13) states that  $\sqrt{P_3(t)}$  can be expanded in a (finite) Fourier series. Thus it is a periodic function with period

$$T = 2\pi\hbar \frac{M}{D} = h \frac{M}{D}. \quad (14)$$

However, this does not mean that spontaneous emission is not present in the system. First, in reality the dimension of space of states is surely huge, possibly infinite. For large  $M$ ,  $T$  is also large. There exists such a big  $M$  that  $T$  is too long to be ever measured. What is more, even when  $T$  is quite small,  $\sqrt{P(t)}$  may be measurably non-zero only for a very short time  $\tau$  in every period. If unavoidable differences in  $t_w$  in different measurements are significantly larger than  $\tau$ , spontaneous emission is observed.

Note that the coefficients of Fourier expansion are dependent only on scalar products of initial state  $|0\rangle$  with eigenstates  $|\tilde{e}_m\rangle$ . The only properties that they must fulfil for all choices of  $\varepsilon_k$  and  $\alpha_k$  are that they are positive real numbers summing to the unity. To prove this we show the algorithm which finds  $\varepsilon_k$  and  $\alpha_k$ :

1. Choose  $|\langle 0|\tilde{e}_m\rangle|^2 > 0$ .  $E_m$  fulfils Eq. (11). In its eigenbasis,  $H$  is a diagonal matrix with elements  $E_m$ .
2.  $|0\rangle$  may be chosen to have real, positive components in the eigenbasis of  $H$ . Their moduli are determined by the choice of  $|\langle 0|\tilde{e}_m\rangle|^2$ .
3. Orthonormalize  $\{|e_{-M}\rangle, \dots, |e_{-1}\rangle, |0\rangle, |e_1\rangle, \dots, |e_M\rangle\}$  using Gram-Schmidt procedure, starting from  $|0\rangle$ . Find  $H$  in this basis.
4. Consider the subspace orthogonal to  $|0\rangle$ . Denote  $H$  reduced to this subspace by  $H_{red}$ . Find the eigenbasis of  $H_{red}$ .
5. Change the basis such, that  $|0\rangle$  stays invariant and the following basis states are eigenstates of  $H_{red}$  extended to the original space. Calculate  $H$  in this basis.
6. The result is the Hamiltonian matrix which has the desired form.

Realizing this algorithm numerically for some concrete  $|\langle 0|\tilde{e}_m\rangle|$  (e.g. in the example considered below) may be an instructive exercise for students.

The corollary is that there exist very wide range of possible  $P(t)$ . For example, we can choose

$$|\langle 0|\tilde{e}_m\rangle|^2 = \frac{1}{2M+1} \quad (15)$$

for any  $m$ . This is not a blind guess. We know, that the Fourier transform of the Dirac delta function is constant, so we expect that with Eq. (15)  $\sqrt{P_3(t)}$  will be considerably different from zero only for  $t$  being close to integer multiple of  $T$ . The results are plotted in Figure 1. It can be seen, how period becomes larger when  $M$  increases. Simultaneously, the time after which the emission happens is approximately independent of  $M$ . Thus for big enough (but still finite)  $M$ , the probability that after long and not precisely determined time  $t_w$  the atom is excited is not measurable.

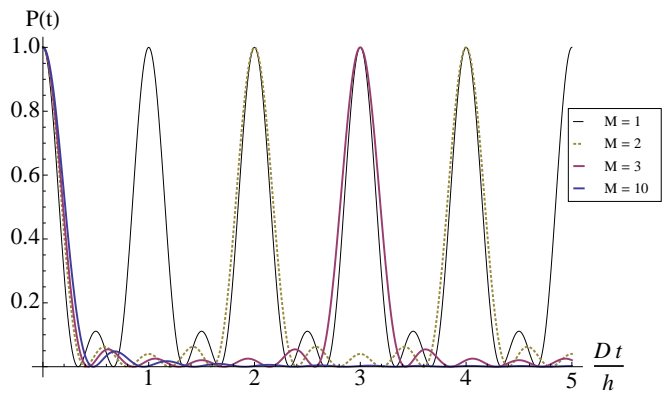


Figure 1: Probability  $P(t)$  that the atom is in excited state after time  $t$  when the relation of the initial state to eigenstates is given by Eq. (15) and the energy eigenvalues are given by Eq. (11). Total number of states equals  $2M+1$ .

## V. CONCLUSIONS OF THE MODEL

We propose a simple quantum model for the system consisted of the two-level atom and  $N$ -modal field. We have shown, that large number of modes is a necessary but (contrary to widespread opinion) not sufficient condition for occurrence of spontaneous emission. Whether the emission is present in the system or not, depends on the interaction with the field and the modes mean energies, which determine the coefficients  $|\langle 0|\tilde{e}_m\rangle|^2$  in Eq. (4).

We have shown the algorithm of building a Hamiltonian which cause  $P(t)$  to be desired function if only square root of this function has a finite expansion in the cosine Fourier series (with any period). This is an extremely broad set of functions. This shows that even a simple two-level atom can undergo various types of an evolution when is placed in a complex environment.

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<sup>1</sup> See for example Zemansky M W, Dittman R H 1997, *Heat and thermodynamics. An intermediate coursebook* 7th edn (McGraw Hill), pp 307-310.

<sup>2</sup> Liboff R L 1980, *Introductory Quantum Mechanics*

(Addison-Wesley); Schiff L I 1968, *Quantum Mechanics* 3rd edn (McGraw-Hill); Bes D 2007, *Quantum Mechanics. A Modern and Concise Introductory Course* (Springer, Berlin Heidelberg).